THERIAK_D Manual

This step-by-step introduction is written to explain the use of the Theriak-Domino add-on “Theriak_D”. We offer two opportunities: a) standard usage with the system shell, and b) usage with MATLAB® or SciLab© programming environment (following the example of the technical brief).

1. Standard Usage:

1.1 Make sure that the Theriak/Domino software package is installed correctly.
See Theriak/Domino Manual:
http://titan.minpet.unibas.ch/minpet/theriak/prog150508/TheriakDominoGuide.pdf

Afterwards copy “theriakd.f90”-file into “TheriakDomino/Programs” directory and replace the “Makefile” with the downloaded version. Then, re-compile the programs:

- Download the gfortran compiler from http://gcc.gnu.org/wiki/GFortranBinaries.
- Install the binaries for gfortran (just double-click the installer and follow the instrucions)
- Open a Terminal (or in Windows a Batch window), make "Programs" the working directory and type:

```
make all
```

1.2 Copy or create an input- and composition-file in your working directory (e.g. “/Users/ theriakd_example”).

1.2.1 The input-file must contain the following information in the following order and format. Example input-file “in”:

`JUN92.bs`	(is the name of database)
`400`	(is temperature in °C)
`5000`	(is pressure in bar)
`DENSOL`	(is the command)

1.2.2 The composition file must have the standard format of Theriak (see “dat-file” in the chapter “Theriak Input files” of Theriak Manual). The dat-file is usually called THERIN or therin.txt. For example, the file “THERIN” contains the following lines:

```
400  2000
0    SI(1)O(2)   *
```

- first line contains the external conditions in the following form:
`temperature(°C)  pressure(bar)`
Theriak_D ignores this line and take the temperature and pressure out of the input-file (see 1.2.1) !

- second line contains:

`0`	(is the print code. Theriak_D ignores the print code)
`SI(1)O(2)`	(is the molar bulk composition)
`*`	(is the user code. In the normal case, an asterisk ***** includes all matching phases)

1.2.3 Make sure that the following files are in your working directory:

a) input-file: “in”
b) composition file: “THERIN”
c) database: “JUN92.bs”

1.3 Start the system shell application (Windows: DOS; Mac: Terminal) and go into your working directory, e.g. type:

```
cd ../theriakd_example
```

1.4 Type in the shell:

```
theriakd in THERIN
```

`theriakd`	(is the command to execute THERIAK_D)
`in`	(is the name of the input-file)
`THERIN`	(is the name of the composition file)

1.5 You will receive an output value in the shell. The value for this explicit example is `2.652988`

2. Example: Usage with MATLAB® or SciLab©

2.1 Download and open the example folder “theriakd_example2”

2.2 Open the script “theriakd.m” (MATLAB®) or “theriakd.sci” (SciLab©).

In line 17, set the path to “theriakd” that is located in your “TheriakDomino/Programs” directory.

In line 19 to 26 (paragraph “LOAD INPUT”) you can chose/insert the desired command, the name of the input-file, the example temperature-, pressure- and model-setup-file. See Table 1 for available commands.

In line 60 to 72, you have the opportunity to change the name of your composition files (usually called “THERIN”, here called “mantle” and “basalt”) and database (usually called “JUN92.bs” or “tcdb55c2d”). Be aware that these files are in the example folder and in the correct format (see point 1.2).

2.3 Run the script

2.4 Wait until calculation is finished

2.5 Watch your results in the opening figure and the array "result"

2.6 You can also load the results of the short note example. Type in the command window of MATLAB®:

`result=load('DENSOL.m')` to load the solid rock density [g/cm^3], or

`result=load('H.m')` to load the amount of hydrogen of free fluids [mol], or

`result=load('GARNET.m')` to load the amount of garnet [mol].

Or type in the Scilab-console of SciLab©:

```
loadmatfile('DENSOL.m');
result=DENSOL
```
to load the solid rock density [g/cm^3], or

```
loadmatfile ('H.m')
result=H
```
to load the amount of hydrogen of free fluids [mol], or

```
loadmatfile ('GARNET.m')
result=GARNET
```
to load the amount of garnet [mol].

Table 1

The table contains all available commands and explanations of Theriak_D. A command should be written in the fourth line of the input-file. Please note that the “DENMELT” and “MMELT” command only work with the tcdb55-database. All other commands function with JUN92.bs and tcdb55-database. Check with the corresponding databases for phase abbreviations and solution names.

DENSOL	total density of solids
VOLSOL	total volume of solids
WTSOL	total molar weight of solids
G	Free Gibbs Energy (System)
H	Hydrogen in free fluid water [mol]
DENH2O	density of free fluid H2O [g/cm3]
H2OSOL	H2O in solids [mol]
WH2OSOL	H2O in solids [g]
WPH2OSOL	H2O in solids [wt%]
*X????$$	Number of moles of an element in a phase [mol]
	???? = First 4 letters of a phase abbreviation or solution
	$$ = element-abbreviation in capital letters
	EXAMPLE 1: *XFo SI = SI in phase 'forsterite' [mol]
	EXAMPLE 2: *XGARNSI = SI in GARNET solution [mol]
*M????	Number of moles of a phases [mol]
	???? = First 4 letters of a phase abbreviation or solution
*W????	Weight percent of a phase [wt%]
	???? = First 4 letters of a phase abbreviation or solution
*V????	Volume percent of a phase [vol%]
	???? = First 4 letters of a phase abbreviation or solution
DENMELT	density of melt [g/cm3]
	(only applicable with tcdb55-database)
MMELT	MELT-Number of moles (Si Al Fe Mg Ca Na K H O)
	(only applicable with tcdb55-database)
KDCTDCAR	KD-value(Fe-Mg) Chloritoid - Carpholite
KDCTDCHL	KD-value(Fe-Mg) Chloritoid - Chlorite
KDGRTBT	KD-value(Fe-Mg) Garnet - Biotite
KDGRTCPX	KD-value(Fe-Mg) Garnet - Clinopyroxene
KDGRTOPX	KD-value(Fe-Mg) Garnet- Orthopyroxene
KDOPXCPX	KD-value(Fe-Mg) Orthopyroxene - Clinopyroxene
KDOLGRT	KD-value(Fe-Mg) Olivine - Garnet
KDOLOPX	KD-value(Fe-Mg) Olivine - Orthopyroxene
KDOLCPX	KD-value(Fe-Mg) Olivine - Clinopyroxene